

(19) World Intellectual Property  
Organization  
International Bureau



(43) International Publication Date  
9 September 2005 (09.09.2005)

PCT

(10) International Publication Number  
**WO 2005/082050 A2**

(51) International Patent Classification: Not classified

(21) International Application Number:  
PCT/US2005/006114

(22) International Filing Date: 24 February 2005 (24.02.2005)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:  
60/546,976 24 February 2004 (24.02.2004) US

(71) Applicant (for all designated States except US): **SSCI, INC.** [US/US]; 3065 Kent Avenue, West Lafayette, IN 47906 (US).

(72) Inventors; and

(75) Inventors/Applicants (for US only): **BATES, Simon** [GB/US]; 3343 Peppermill Drive, West Lafayette, IN 47906 (US). **IVANISEVIC, Igor** [HR/US]; 3317 Secretariat Circle, West Lafayette, IN 47906 (US).

(74) Agent: **GARRETT, Arthur, S.**; Finnegan, Henderson, Farabow, Garrett & Dunner, L.L.P., 901 New York Avenue, NW, Washington, DC 20001 (US).

(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

**Published:**

— without international search report and to be republished upon receipt of that report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: ANALYSIS AND SCREENING OF SOLID FORMS USING THE ATOMIC PAIR DISTRIBUTION FUNCTION

(57) Abstract: A method that comprises providing a PDF trace of a first sample of a substance, providing a PDF trace of a second sample of the substance, and comparing the PDF traces to determine whether the substance of the first sample and the substance of the second sample have the same or different solid forms. This embodiment may be used, for example, to distinguish one solid form of a compound from another, to screen for new solid forms of a compound, or to determine whether a disordered crystalline compound has the same solid form as another crystalline sample of the compound.



WO 2005/082050 A2